CHAPTER 9 – Molecular Geometry and Bonding Theories

Section 9.1 – Molecular Shapes

(a) A student drew a Lewis structure for carbon tetrachloride and concluded that the bond angles in the CCl_4 molecule must be 90^o. Do you agree? If not, draw an accurate representation of the molecule and identify what the bond angles should be.

(b) Do you predict that the bond length in carbon tetrafluoride should be shorter than, longer than, or the same as the bond length in carbon tetrachloride? Justify your prediction.

(c) The shape of the CO_2 molecule is __________________ and has a bond angle of _________.

(d) Identify the shape of the SO_2 molecule, which is not the same as that of the CO_2 molecule. Justify your answer based on the Lewis structure for SO_2.

(e) The shape of the SO_3 molecule is _________________________, and it has bond

angles of ____________.

(f) The shape of the CH_4 molecule is _________________________, and it has bond

angles of ____________.

(g) The shape of the PF_5 molecule is __________________________, and it has bond

angles of _________ and _________.

(h) The shape of the SF_6 molecule is __________________________, and it has bond

angles of ____________.

(i) Draw the Lewis structure for each of the following molecules. Then identify the shape and the bond angles in the molecule. See Figure 9.3 on page 333 for examples.

carbon disulfide	arsenic pentachloride
boron trifluoride	selenium hexafluoride
silicon tetrabromide	

(j) What does VSEPR stand for?

Section 9.2 – The VSEPR Model

(a) An electron domain can consist of either a _______________ pair or a ___________________ pair of electrons. Each multiple bond in a molecule also constitutes a single electron domain.

(b) The VSEPR model is based on the idea that electron domains are negatively charged and therefore _______________ one another. The best arrangement of a given number of electron domains is the one that ____

(c) What is the difference between electron domain geometry and molecular geometry? Use the water molecule as an example to explain the difference between the two.

(d) For each of the following molecules, count the bonding and nonbonding electron domains around the central atom. Identify both the electron domain geometry and the molecular geometry.

Molecule	Bonding Domains around central atom	Nonbonding Domains around central atom	Total # of Electron Domains around central atom	Electron Domain Geometry	Molecular Geometry
CO_2					
BH_3					
O_3					
CH_4					
NH_3					
H_2O					

(e) Fill in the information in the table below. For the examples in the right side of the table, select from the following list of molecules and ions. Use Table 9.2 on page 337 to help you.

SO_2 SCl_2 SO_3 PCl_3 CCl_4 HCN

NO_2^- ClO_2^- NO_3^- ClO_3^- SO_4^{2-} N_3^-

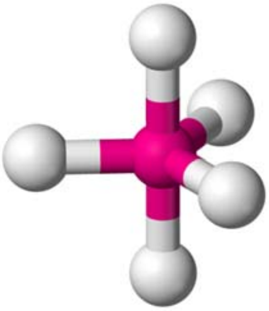
Total # of Electron Domains around central atom	Electron Domain Geometry	Bonding Domains around central atom	Nonbonding Domains around central atom	Molecular Geometry	Example of a Molecule	Example of a Poly-atomic Ion
2		2	0			
3		3	0			
		2	1			
4		4	0			
		3	1			
		2	2			

(f) Explain why the bond angles in NH_3 and H_2O are less than 109.5°.

(g) Explain why the Cl–C–Cl bond angle in phosgene ($Cl_2C=O$) is less than 120°.

(h) Molecules with five or six electron domains around the central atom have molecular geometries based on either a ________________________________ (five domains) or _____________________ (six domains) electron domain geometry.

(i) Label the axial and the equatorial positions on the molecule shown below.



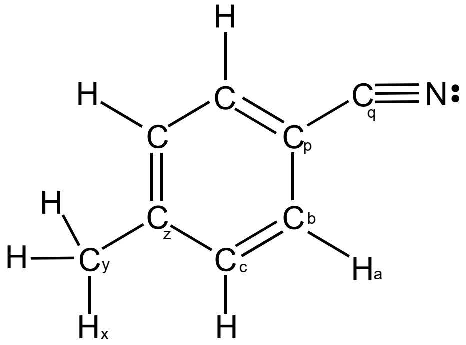
(j) Because the domains from nonbonding pairs exert __________________ repulsions than those from bonding pairs, nonbonding domains always occupy the ______________________ positions in a trigonal bipyramid.

(k) Fill in the information in the table below. For the examples in the right side of the table, select from the following list of molecules and ions. Use Table 9.3 on page 340 to help you.

XeF_2 ClF_3 XeF_4 SF_4 ClF_5 PF_5 SF_6

Br_3^- PF_4^- IF_4^- SF_5^+ PF_6^-

Total # of Electron Domains around central atom	Electron Domain Geometry	Bonding Domains around central atom	Nonbonding Domains around central atom	Molecular Geometry	Example of a Molecule	Example of a Poly-atomic Ion
5		5	0			
		4	1			
		3	2			N/A
		2	3			
6		6	0			
		5	1			N/A
		4	2			



(l) Based on the molecule shown above and your knowledge of the VSEPR model, predict the bond angle for each of the following bonds.

$H_x – C_y – C_z$ __________

$H_a – C_b – C_c$ __________

$C_p – C_q – N$ __________

Section 9.3 – Molecular Shape and Molecular Polarity

(a) The C–O bond and the H–O bond are polar bonds because ______________________________

____

(b) The CO_2 molecule is nonpolar because ____

____

(c) The H_2O molecule is polar because ____

____

(d) Identify the shape of each molecule and classify it as polar or nonpolar.

Molecule	Bonding Domains around central atom	Nonbonding Domains around central atom	Molecular Geometry	Polar or Nonpolar?
CO_2				
HCN				
BF_3				
CCl_2O				
SO_2				
CH_4				
CH_3Cl				
NH_3				
H_2O				
PF_5				
PF_4Cl				
SF_4				
ClF_3				
XeF_2				
SF_6				
BrF_5				
XeF_4				

Section 9.4 – Covalent Bonding and Orbital Overlap

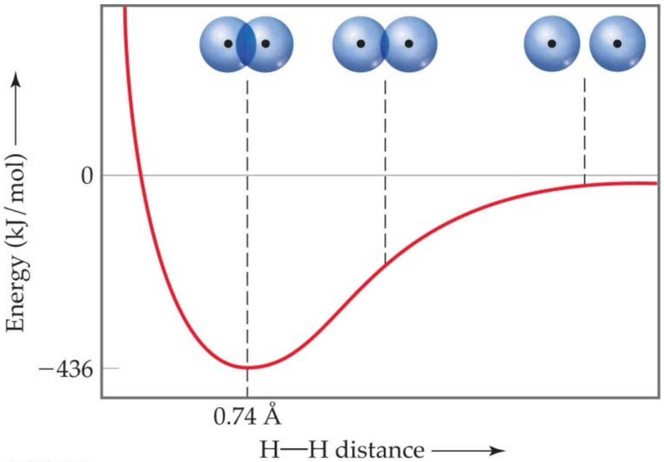
(a) The ________________ of orbitals allows two electrons of opposite spin to share the space between the nuclei, forming a ____________________________

(b) In the H_2 molecule, what type of orbitals overlap to form a bond? ________________

(c) In the Cl_2 molecule, what type of orbitals overlap to form a bond? ________________

(d) In the HCl molecule, what type of orbitals overlap to form a bond? ________________

Refer to the diagram at right, which is Figure 9.14 on page 346.



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(e) When the two H atoms are very far apart, the potential energy approaches what value? ____________________

(f) As the two H atoms move closer together, the potential energy ________________ as the strength of the bond ________________.

(g) When the distance between the two H atoms becomes less than 0.74 Å, the potential energy ____________________ because of the ____

(h) The observed ______________________ is the distance at which the ____________________ forces between unlike charges (electrons and nuclei) are balanced by the ________________ forces between like charges (electron-electron and nucleus-nucleus)

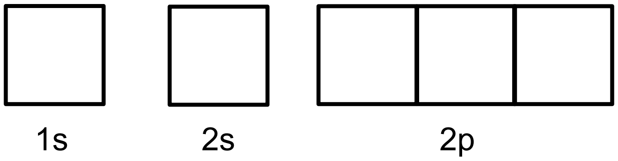
Section 9.5 – Hybrid Orbitals

(a) To explain molecular geometries, we can assume that the atomic orbitals on an atom (usually the central atom) _______________ to form new orbitals called _________________ orbitals.

(b) The process of mixing atomic orbitals is a mathematical operation called

____

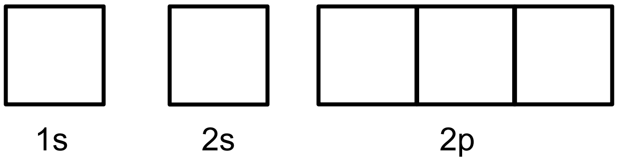
(c) Fill in the arrows in the orbital diagram for the ground state configuration of beryllium.



(d) The Be atom in its ground state cannot bond with the fluorine atoms because it has no

____

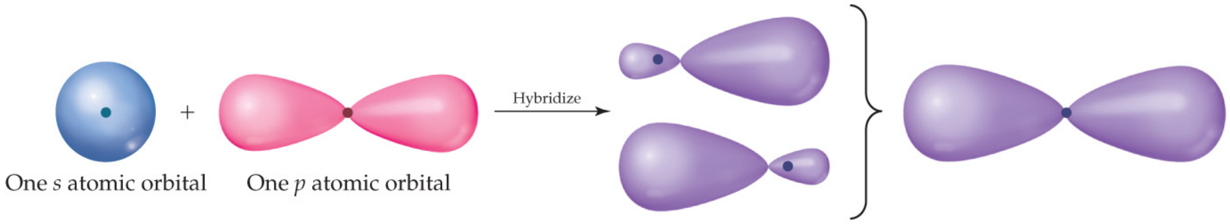
(e) The Be atom could form two bonds by “promoting” one of the 2s electrons to a 2p orbital. Fill in the orbital diagram for this configuration of beryllium that has two unpaired electrons.



(f) The Be atom now has two unpaired electrons and can form two covalent bonds with fluorine atoms. However, the two bonds would not be ________________________, because one of the bonds would involve a _________ orbital and the other bond would involve a _________ orbital.

(g) We can solve this dilemma by “mixing” the 2s orbital with one 2p orbital. The result is the creation of two new identical hybrid orbitals called _________ orbitals.

(See Figure 9.15 on page 347.)



(h) See Figure 9.16 on page 347. In the diagram below, draw the two large lobes of the sp hybrid orbitals and show how they overlap with the 2p orbitals of fluorine to form two polar covalent bonds.

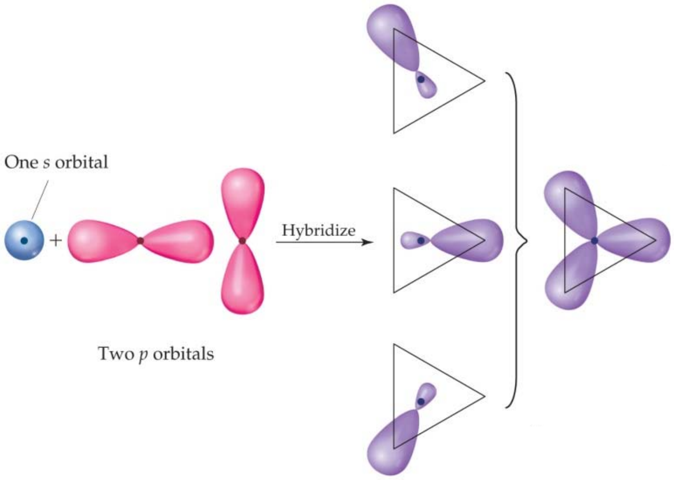
(i) According to the valence-bond model, a ____________________ arrangement of electron domains implies sp hybridization.

(j) Fill in the orbital diagram for the ground state configuration of boron.

☐ ☐ ☐☐☐

1s 2s 2p

(k) We have a similar problem as we did with beryllium. The ground-state electron configuration of boron does not have three unpaired electrons. Just like with Be, we can solve this dilemma with B by "mixing" the 2s orbital with two of the 2p orbitals. The result is the creation of three new identical hybrid orbitals called ________ orbitals.
(See Figure 9.17 on page 348.)

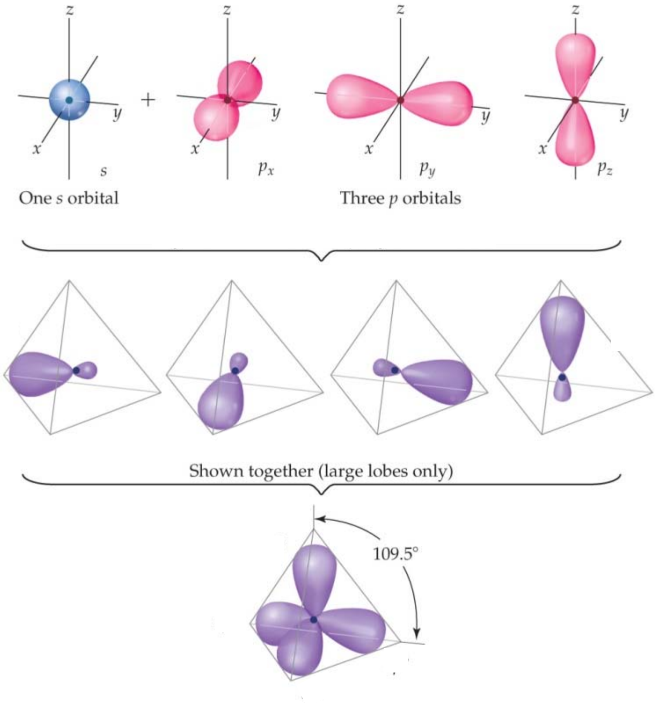


(l) According to the valence-bond model, a ___________________________ arrangement of electron domains implies sp^2 hybridization.

(m) Fill in the orbital diagram for the ground state configuration of carbon.

☐ ☐ ☐☐☐

(n) We have a similar problem as we did with beryllium and boron. The ground-state electron configuration of carbon does not have four unpaired electrons. We can solve this dilemma by "mixing" the 2s orbital with the three 2p orbitals. The result is the creation of four new identical hybrid orbitals called ________ orbitals.
(See Figure 9.18 on page 349.)



(o) According to the valence-bond model, a ____________________________ arrangement of electron domains implies sp^3 hybridization.

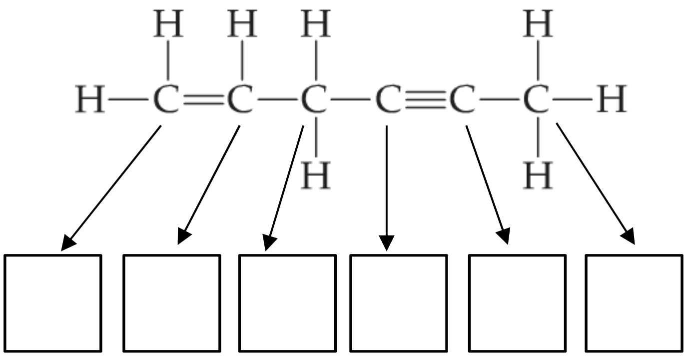
(p) Identify the orbital hybridization around the central atom in each of the following.

BeF_2 ________ CCl_2O ________ NH_3 ________

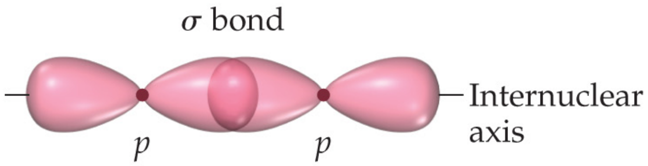
BF_3 _________ SiH_4 __________ H_2O ________

CF_4 _________ CO_2 __________ O_3 __________

(q) Identify the orbital hybridization for each carbon atom in the following molecule.



Section 9.6 – Multiple Bonds



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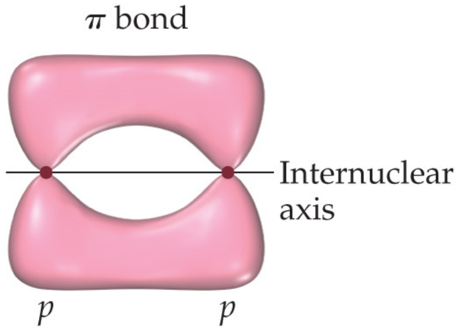
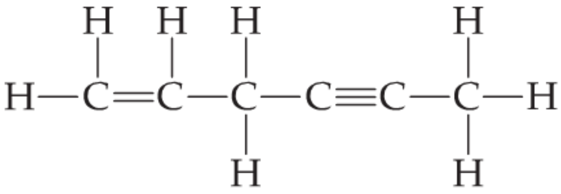


(a) A bond in which the electron density is concentrated along the line connecting the nuclei (the internuclear axis) is called a ____________________ bond.

(b) To describe multiple bonding, we must consider a second kind of bond. This one is the result of the overlap between two p orbitals oriented perpendicularly to the internuclear axis. This sideways overlap of p orbitals produces a ________________ bond.

(c) In almost all cases, single bonds are _________________ bonds. A double bond consists of one _____________ bond and one ___________ bond. A triple bond consists of one _____________ bond and two ___________ bonds.

(d) How many sigma (σ) and pi (π) bonds are present in the following molecule?

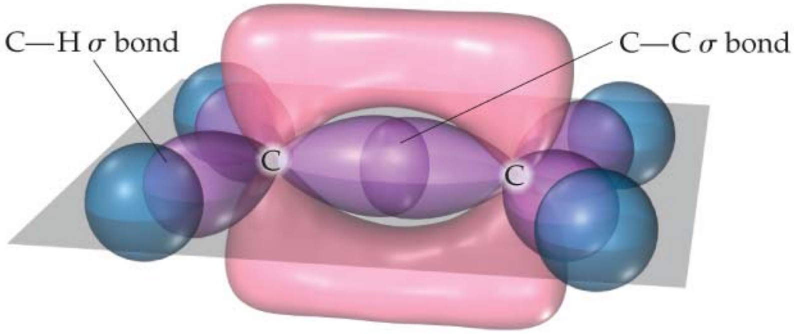


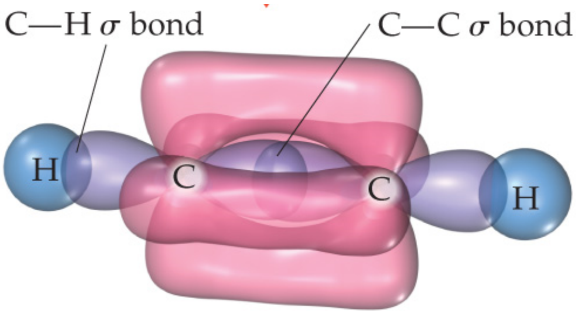
$H-C=C-C-C\equiv C-C-H$

_______ sigma (σ) bonds

_______ pi (π) bonds

(e) Label the pi (π) bonds on the following diagrams of ethylene (C_2H_4) and acetylene (C_2H_2).





(f) For molecules that contain two or more resonance structures involving π bonds, we cannot describe the π bonds as individual bonds between neighboring atoms. Therefore we say that the π bonds are ________________________, or spread out among several atoms involved in the resonance structures.

Section 9.7 – Molecular Orbitals

Section 9.8 – Period 2 Diatomic Molecules

Molecular orbitals are beyond the scope of this course and the AP Exam. They will not be covered.